

Table S1. High-resolution structures of archaeal virus proteins.

PDB ID	Virus name	Protein name	Function	Fold	References
<i>Fuselloviridae</i>					
4LID	SSV1	A100	Essential protein conserved in fuselloviruses	Novel $\alpha\beta$ fold	Unpublished
2WBT	SSV1	B129	Putative DNA-binding protein	Double C2H2 zinc finger	Unpublished
3VCF, 4DKS, 3UXU	SSV1	D335	Tyrosine recombinase	α/β integrase fold	(Eilers et al., 2012; Zhan et al., 2012)
1SKV	SSV1	D63	Putative adaptor protein	Four-helix bundle, dimer	(Kraft et al., 2004a)
2W8M	SSV-RH	D212	Putative Holliday junction resolvase	PD-(D/E)XK fold	(Menon et al., 2010)
4AAI	SSV-RH	E73	Putative transcription regulator	RHH	(Schlenker et al., 2012)
1TBX	SSV1	F93	Putative transcription regulator	wHTH	(Kraft et al., 2004b)
2VQC	SSV1	F112	Putative transcription regulator	wHTH	(Menon et al., 2008)
<i>Bicaudaviridae</i>					
4ART, 4ATS	ATV	ORF273	Structural protein	Novel $\alpha\beta$ fold	(Felisberto-Rodrigues et al., 2012)
3FAJ	ATV	P131	Major structural protein	Four-helix bundle	(Goulet et al., 2010b)
5EQW	ATSV	D135	Major structural protein	Four-helix bundle	(Hochstein et al., 2015)
<i>Rudiviridae</i>					
2X48	SIRV1	ORF55	DNA-binding protein	wHTH	(Oke et al., 2010)
2KEL	SIRV1	ORF56b	transcriptional regulator SvtR	RHH	(Guilliere et al., 2009)
2X4I	SIRV1	ORF114a	Unknown, DNA-binding protein	Novel $\alpha\beta$ fold	(Oke et al., 2010)
2X3G	SIRV1	ORF119	Rep protein	α/β RCRE fold	(Oke et al., 2010; Oke et al., 2011)
2X5T, 2X5G, 2X5H	SIRV1	ORF131	ssDNA-binding protein	Novel $\alpha\beta$ fold	(Oke et al., 2010)
3J9X	SIRV2	ORF134	Major capsid protein	α -helical bundle	(DiMaio et al., 2015)
3F2E	SIRV-YNP	MCP	Major capsid protein	α -helical bundle	(Szymczynska et al., 2009)
<i>Lipothrixviridae</i>					
2LVH	AFV1	ORF59a	DNA binding, putative transcription regulator	C2H2 zinc finger	(Guilliere et al., 2013)
3DF6, 3DJW	AFV1	ORF99	Unknown	Novel $\alpha\beta$ fold	(Goulet et al., 2009b)
2WB6	AFV1	ORF102	Putative macromolecular binding protein	Novel $\beta/\alpha/\beta$ sandwich	(Keller et al., 2009)
5W7G_B, 3FBL	AFV1	ORF132	Major capsid protein 1	α -helical bundle	(Goulet et al., 2009a; Kasson et al., 2017)
5W7G_A, 3FBZ	AFV1	ORF140	Major capsid protein 2	α -helical bundle	(Goulet et al., 2009a; Kasson et al., 2017)
3II2, 3II3, 3ILD, 3ILE	AFV1	ORF157	Nuclease	$\alpha\beta$ nucleotidyltransferase fold	(Goulet et al., 2010a)
2J6B, 2J6C	AFV3	ORF109	Unknown, DNA-binding protein	Novel $\alpha\beta$ fold	(Keller et al., 2007)
4HV0	AFV6	gp29	Transcriptional regulator AvtR	RHH	(Peixeiro et al., 2013)
2H36	SIFV	SIFV0014	Unknown	Novel $\alpha\beta$ fold	(Goulet et al., 2009b)
<i>Globuloviridae</i>					
2X5R	PSV	ORF126	Unknown	Novel fold	(Oke et al., 2010)
2X5C	PSV	ORF131	Unknown	Novel fold	(Oke et al., 2010)
2X4J	PSV	ORF137	Putative archaeal Hfq-like protein	α/β Sm/Hfq fold	(Oke et al., 2010)
2X3M	PSV	ORF239	Unknown	Novel fold	(Oke et al., 2010)
2VXZ	PSV	ORF165a	Putative transcriptional regulator	wHTH	(Oke et al., 2010)
<i>Turriviridae</i>					
3RKL	STIV	A81	Unknown	Novel $\alpha\beta$ fold	Unpublished
2C0N	STIV	A197	Glycosyltransferase	$\alpha/\beta/\alpha$ sandwich	(Larson et al., 2006)
4IL7	STIV	A223	Structural protein, penton base	Triple jelly roll fold	(Veesler et al., 2013)
2J85	STIV	B116	Unknown, DNA-binding protein	Novel $\alpha\beta$ fold	(Larson et al., 2007b)
4R2H, 4R2I	STIV	B204	Genome packaging ATPase	FtsK-HerA fold	(Dellas et al., 2015)
2BBD, 3J31	STIV	B345	Major capsid protein	Double β -barrel	(Khayat et al., 2005; Veesler et al., 2013)
4IND	STIV	C381	Structural protein, turret	Triple jelly roll fold	(Veesler et al., 2013)
2CO5	STIV	F93	Putative transcriptional regulator	wHTH	(Larson et al., 2007a)

4KFR, 4KFS, 4KFT, 4KFU	STIV2	B204	Genome packaging ATPase	FtsK-HerA fold	(Happonen et al., 2013)
<i>Clavaviridae</i> 50XE	APBV1	VP1	Major capsid protein	Novel, α -helical hairpin	(Ptchelkine et al., 2017)
Unclassified 4HR1	PAV1	ORF137	Unknown. predicted involvement in protein-protein/DNA interactions	Four-helix bundle	(Leulliot et al., 2013)

Abbreviations: (w)HTH, (winged) helix-turn-helix; RHH, ribbon-helix-helix; RCRE, rolling circle replication initiation endonuclease. The table is updated from (Dellas et al., 2014).

References

- Dellas, N., Snyder, J.C., Bolduc, B., Young, M.J., 2014. Archaeal Viruses: Diversity, Replication, and Structure. *Annu Rev Virol* 1(1), 399-426.
- Dellas, N., Snyder, J.C., Dills, M., Nicolay, S.J., Kerchner, K.M., Brumfield, S.K., Lawrence, C.M., Young, M.J., 2015. Structure-Based Mutagenesis of *Sulfolobus* Turreted Icosahedral Virus B204 Reveals Essential Residues in the Virion-Associated DNA-Packaging ATPase. *J Virol* 90(6), 2729-2739.
- DiMaio, F., Yu, X., Rensen, E., Krupovic, M., Prangishvili, D., Egelman, E.H., 2015. Virology. A virus that infects a hyperthermophile encapsidates A-form DNA. *Science* 348(6237), 914-917.
- Eilers, B.J., Young, M.J., Lawrence, C.M., 2012. The structure of an archaeal viral integrase reveals an evolutionarily conserved catalytic core yet supports a mechanism of DNA cleavage in trans. *J Virol* 86(15), 8309-8313.
- Felisberto-Rodrigues, C., Blangy, S., Goulet, A., Vestergaard, G., Cambillau, C., Garrett, R.A., Ortiz-Lombardia, M., 2012. Crystal structure of ATV(ORF273), a new fold for a thermo- and acido-stable protein from the *Acidianus* two-tailed virus. *PLoS One* 7(10), e45847.
- Goulet, A., Blangy, S., Redder, P., Prangishvili, D., Felisberto-Rodrigues, C., Forterre, P., Campanacci, V., Cambillau, C., 2009a. *Acidianus* filamentous virus 1 coat proteins display a helical fold spanning the filamentous archaeal viruses lineage. *Proc Natl Acad Sci U S A* 106(50), 21155-21160.
- Goulet, A., Pina, M., Redder, P., Prangishvili, D., Vera, L., Lichiere, J., Leulliot, N., van Tilbeurgh, H., Ortiz-Lombardia, M., Campanacci, V., Cambillau, C., 2010a. ORF157 from the archaeal virus *Acidianus* filamentous virus 1 defines a new class of nuclease. *J Virol* 84(10), 5025-5031.
- Goulet, A., Spinelli, S., Blangy, S., van Tilbeurgh, H., Leulliot, N., Basta, T., Prangishvili, D., Cambillau, C., Campanacci, V., 2009b. The thermo- and acido-stable ORF-99 from the archaeal virus AFV1. *Protein Sci* 18(6), 1316-1320.
- Goulet, A., Vestergaard, G., Felisberto-Rodrigues, C., Campanacci, V., Garrett, R.A., Cambillau, C., Ortiz-Lombardia, M., 2010b. Getting the best out of long-wavelength X-rays: de novo chlorine/sulfur SAD phasing of a structural protein from ATV. *Acta Crystallogr D Biol Crystallogr* 66(Pt 3), 304-308.
- Guilliere, F., Danioux, C., Jaubert, C., Desnoues, N., Delepierre, M., Prangishvili, D., Sezonov, G., Guijarro, J.I., 2013. Solution structure of an archaeal DNA binding protein with an eukaryotic zinc finger fold. *PLoS One* 8(1), e52908.
- Guilliere, F., Peixeiro, N., Kessler, A., Raynal, B., Desnoues, N., Keller, J., Delepierre, M., Prangishvili, D., Sezonov, G., Guijarro, J.I., 2009. Structure, function, and targets of the transcriptional regulator SvtR from the hyperthermophilic archaeal virus SIRV1. *J Biol Chem* 284(33), 22222-22237.
- Happonen, L.J., Oksanen, E., Liljeroos, L., Goldman, A., Kajander, T., Butcher, S.J., 2013. The structure of the NTPase that powers DNA packaging into *Sulfolobus* turreted icosahedral virus 2. *J Virol* 87(15), 8388-8398.
- Hochstein, R., Bollsweiler, D., Engelhardt, H., Lawrence, C.M., Young, M., 2015. Large Tailed Spindle Viruses of Archaea: a New Way of Doing Viral Business. *J Virol* 89(18), 9146-9149.
- Kasson, P., DiMaio, F., Yu, X., Lucas-Staat, S., Krupovic, M., Schouten, S., Prangishvili, D., Egelman, E.H., 2017. Model for a novel membrane envelope in a filamentous hyperthermophilic virus. *eLife* 6, e26268.
- Keller, J., Leulliot, N., Cambillau, C., Campanacci, V., Porciero, S., Prangishvili, D., Forterre, P., Cortez, D., Quevillon-Cheruel, S., van Tilbeurgh, H., 2007. Crystal structure of AFV3-109, a highly conserved protein from crenarchaeal viruses. *Virol J* 4, 12.
- Keller, J., Leulliot, N., Collinet, B., Campanacci, V., Cambillau, C., Prangishvili, D., van Tilbeurgh, H., 2009. Crystal structure of AFV1-102, a protein from the *acidianus* filamentous virus 1. *Protein Sci* 18(4), 845-849.

- Khayat, R., Tang, L., Larson, E.T., Lawrence, C.M., Young, M., Johnson, J.E., 2005. Structure of an archaeal virus capsid protein reveals a common ancestry to eukaryotic and bacterial viruses. *Proc Natl Acad Sci U S A* 102(52), 18944-18949.
- Kraft, P., Kummel, D., Oeckinghaus, A., Gauss, G.H., Wiedenheft, B., Young, M., Lawrence, C.M., 2004a. Structure of D-63 from *Sulfolobus* spindle-shaped virus 1: surface properties of the dimeric four-helix bundle suggest an adaptor protein function. *J Virol* 78(14), 7438-7442.
- Kraft, P., Oeckinghaus, A., Kummel, D., Gauss, G.H., Gilmore, J., Wiedenheft, B., Young, M., Lawrence, C.M., 2004b. Crystal structure of F-93 from *Sulfolobus* spindle-shaped virus 1, a winged-helix DNA binding protein. *J Virol* 78(21), 11544-11550.
- Larson, E.T., Eilers, B., Menon, S., Reiter, D., Ortmann, A., Young, M.J., Lawrence, C.M., 2007a. A winged-helix protein from *Sulfolobus* turreted icosahedral virus points toward stabilizing disulfide bonds in the intracellular proteins of a hyperthermophilic virus. *Virology* 368(2), 249-261.
- Larson, E.T., Eilers, B.J., Reiter, D., Ortmann, A.C., Young, M.J., Lawrence, C.M., 2007b. A new DNA binding protein highly conserved in diverse crenarchaeal viruses. *Virology* 363(2), 387-396.
- Larson, E.T., Reiter, D., Young, M., Lawrence, C.M., 2006. Structure of A197 from *Sulfolobus* turreted icosahedral virus: a crenarchaeal viral glycosyltransferase exhibiting the GT-A fold. *J Virol* 80(15), 7636-7644.
- Leulliot, N., Quevillon-Cheruel, S., Graille, M., Geslin, C., Flament, D., Le Romancer, M., van Tilbeurgh, H., 2013. Crystal structure of PAV1-137: a protein from the virus PAV1 that infects *Pyrococcus abyssi*. *Archaea* 2013, 568053.
- Menon, S.K., Eilers, B.J., Young, M.J., Lawrence, C.M., 2010. The crystal structure of D212 from *Sulfolobus* spindle-shaped virus ragged hills reveals a new member of the PD-(D/E)XK nuclease superfamily. *J Virol* 84(12), 5890-5897.
- Menon, S.K., Maaty, W.S., Corn, G.J., Kwok, S.C., Eilers, B.J., Kraft, P., Gillitzer, E., Young, M.J., Bothner, B., Lawrence, C.M., 2008. Cysteine usage in *Sulfolobus* spindle-shaped virus 1 and extension to hyperthermophilic viruses in general. *Virology* 376(2), 270-278.
- Oke, M., Carter, L.G., Johnson, K.A., Liu, H., McMahon, S.A., Yan, X., Kerou, M., Weikart, N.D., Kadi, N., Sheikh, M.A., Schmelz, S., Dorward, M., Zawadzki, M., Cozens, C., Falconer, H., Powers, H., Overton, I.M., van Niekerk, C.A., Peng, X., Patel, P., Garrett, R.A., Prangishvili, D., Botting, C.H., Coote, P.J., Dryden, D.T., Barton, G.J., Schwarz-Linek, U., Challis, G.L., Taylor, G.L., White, M.F., Naismith, J.H., 2010. The Scottish Structural Proteomics Facility: targets, methods and outputs. *J Struct Funct Genomics* 11(2), 167-180.
- Oke, M., Kerou, M., Liu, H., Peng, X., Garrett, R.A., Prangishvili, D., Naismith, J.H., White, M.F., 2011. A dimeric Rep protein initiates replication of a linear archaeal virus genome: implications for the Rep mechanism and viral replication. *J Virol* 85(2), 925-931.
- Peixeiro, N., Keller, J., Collinet, B., Leulliot, N., Campanacci, V., Cortez, D., Cambillau, C., Nitta, K.R., Vincentelli, R., Forterre, P., Prangishvili, D., Sezonov, G., van Tilbeurgh, H., 2013. Structure and function of AvtR, a novel transcriptional regulator from a hyperthermophilic archaeal lipothrixvirus. *J Virol* 87(1), 124-136.
- Ptchelkine, D., Gillum, A., Mochizuki, T., Lucas-Staat, S., Liu, Y., Krupovic, M., Phillips, S., Prangishvili, D., Huiskonen, J., 2017. Unique architecture of thermophilic archaeal virus APBV1 and its genome packaging. *Nat Commun* 8, 1436.
- Schlenker, C., Goel, A., Tripet, B.P., Menon, S., Willi, T., Dlakic, M., Young, M.J., Lawrence, C.M., Copie, V., 2012. Structural studies of E73 from a hyperthermophilic archaeal virus identify the "RH3" domain, an elaborated ribbon-helix-helix motif involved in DNA recognition. *Biochemistry* 51(13), 2899-2910.
- Szymczyzna, B.R., Taurog, R.E., Young, M.J., Snyder, J.C., Johnson, J.E., Williamson, J.R., 2009. Synergy of NMR, computation, and X-ray crystallography for structural biology. *Structure* 17(4), 499-507.
- Veesler, D., Ng, T.S., Sendamarai, A.K., Eilers, B.J., Lawrence, C.M., Lok, S.M., Young, M.J., Johnson, J.E., Fu, C.Y., 2013. Atomic structure of the 75 MDa extremophile *Sulfolobus* turreted icosahedral virus determined by CryoEM and X-ray crystallography. *Proc Natl Acad Sci U S A* 110(14), 5504-5509.
- Zhan, Z., Ouyang, S., Liang, W., Zhang, Z., Liu, Z.J., Huang, L., 2012. Structural and functional characterization of the C-terminal catalytic domain of SSV1 integrase. *Acta Crystallogr D Biol Crystallogr* 68(Pt 6), 659-670.